Computation and parameterization of normalized glandular dose using Geant4[*]

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The average absorbed dose in glandular tissue is the most appropriate parameter for the assessment of the radiation-induced risk during breast imaging. The aims of this work concern: (1) the investigation of the variation effect of any related update to photon cross-section data-bases on the computation of the normalized glandular dose (DgN) for mammography quality control tests and (2) the proposition of a parameterization method leading to provide DgN values function of the breast thickness (T) and the particle energy (E) instead of E alone, as normally known. We analyzed the change effect of the photon cross-section data-bases on the computation of DgN. Those coefficients, generated using the Geant4 Monte Carlo toolkit, were studied over a range of compressed breast thickness of 2–8 cm for monoenergetic (1–120 keV by 1 keV intervals) and polyenergetic (23–35 kVp by 2 kVp intervals) X-ray beams. Moreover, breast tissue composition ranging from about 0% glandular (about 100% adipose) to 100% glandular (0% adipose) was also covered. The successful parameterization of DgN look-up table function of the breast thickness and energy, will compact its analytical form without loss of accuracy. All parameterization fits resulted in r^2 values of 0.999 or better.

Keywords: Monte Carlo simulation, Geant4, Normalized glandular dose, Parameterization

I. INTRODUCTION

Since the glandular breast tissue is regarded as the most radio-sensitive tissue, breast dosimetry has been considered as an important basis for assessment of radiation risk of patients undergoing mammography [1]. The average absorbed dose in the glandular breast tissue, known as the mean glandular dose (*MGD*), is preferred for radiation risk assessment. It can be estimated by measuring the entrance air kerma and by using normalized glandular dose (*DgN*) conversion coefficients for a given breast thickness and glandularity [2].

Among the most prominent factors influencing *DgN* values was the photon fluence per exposure factor (photon quanta per mm^2 per mR). Such factor depends on the mass energy absorption coefficient tables for air (μ_{en}/ρ) which can be extracted from existing data bases, i.e. MCPLIB [3], XCOM [4]. Moreover, the use of MCPLIB cross section leads to 10% higher conversion coefficient values than the use of XCOM data, as pointed out by Zoetelief *et al.* [2]. Thus, the need to update existing monoenergetic *DgN(E)*, look-up tables reveals importance for any occurring change in the (μ_{en}/ρ) tables, and the immediately dependent Monte Carlo simulation programs used to generate such data.

On the other hand, due to the large amount of tabulated *DgN* values used for optimizing mammographic procedures, provided by many authors [5–10], the requirement of parameterization is obvious in order to simplify direct calculation of *MGD* after measuring the incident air kerma. Thus, we can refer to many works focused on that issue [11–13]. Nevertheless, introduction of breast thickness as a second parameter other than energy for parameterization of data-bases does not seem well studied, which can lead to more generalizing the fitting equations.

In this paper, we study effect of the photon fluence per exposure parameter on the calculation of *DgN* values; fact that seems essential after observation of variation of (μ_{en}/ρ) values between the derived data from Hubbel *et al.* [14] and those used by Boone *et al.* [11]. The data of monoenergetic *DgN* conversion coefficients are parameterized so that simple custom function can be easily handled on a spreadsheet to calculate *DgN* values for a given set of input parameters (photon energy, breast composition and thickness). Then, we adopt a mathematical fitting method, where we include the breast thickness as a second parameter and compare their accuracy to predict direct computational results. Finally, we check ability of the method to expect *MGD* for clinically relevant study cases, as carried out by many authors [15], of X-ray tube anode/filter combinations of Mo/Mo (30 μm), W/Rh (50 μm) and W/Pd (50 μm), 23–35 kVp, breast thickness of 4 cm and glandularity of 50%. This work can be considered as a continuation of many recent works around the *MGD* calculation topic [16–18], performed by medical physicist as part of mammography quality control tests.

II. MATERIALS AND METHODS

There are many Monte Carlo simulation packages that can be used for estimating the *MGD*, with different advantages and disadvantages. Accurate and versatile general-purpose simulation packages such as Geant3 [19], EGS4 [20], MCNP [21] and most recently Geant4 [22] include well validated physics models, geometry-modeling tools and efficient

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visualization utilities and do not require any additional effort to be tailored for medical imaging application. For the current study we proceed with the Geant4 toolkit.

To afford an updated data set of *DgN* coefficients for mammography, covering the energy interval of 1–120 keV, for thicknesses of 2–8 cm and glandularities (0%–100%) of compressed breast, we considered the same experimental set-up used by Boone *et al.* [11]. The studied energy interval gives the possibility of using look-up tables for standard (up to 40 kVp) and dual-energy (up to 120 kVp) mammography imaging. We developed a Monte Carlo simulation program to generate the data. Mathematical fitting procedure was followed to parameterize the large amount of data.

According Refs. [1, 23, 24], the *MGD* calculation is highly influenced by spatial distribution of glandular tissues within the breast. Thus, the current study is dedicated to further enhance the quality assurance and quality control procedures involving equipment performance, comparisons of X-ray machines efficiency and mammography dosimetry protocols.

For possible larger compressed breast thickness of 8 cm, the same parameterization procedure should be followed with the penalty of complicating equation and some extra fitting parameters will be needed.

A. Simulation procedure

In order to derive $DgN(E)$ values, we used the photon quanta per mm^2 per mR parameter, $K(E)$, for a given energy E (in keV) of incident photon beam in a medium of air as derived by Johns *et al.* [25]

$$K(E) = 54\,300/[E(\mu_{en}/\rho)_{air}], \qquad (1)$$

where, $(\mu_{en}/\rho)_{air}$, in cm^2/g, is the mass energy absorption coefficient in air.

The $DgN(E)$ coefficient, in mGy/mGy, is given by [26, 27]

$$DgN(E) = \frac{1.8352 \times 10^{-17} E_{dep} G(E) K(E)}{f_g \rho (T - 2T_{skin})(R_2/R_1)^2}, \qquad (2)$$

where, E_{dep} is the energy deposited in the breast tissue, f_g is the glandular fraction of the breast, ρ is the breast density, $R_1 = 8$ cm is breast radius, $R_2 = 7.6$ cm is breast tissue radius excluding the skin, T_{skin} is the skin thickness, T is the breast thickness and $G(E)$ is a factor describing the proportion of the absorbed dose of glandular tissue to the overall breast tissues and given by

$$G(E) = \frac{f_g (\mu_{en}/\rho)_g}{f_g (\mu_{en}/\rho)_g + (1 - f_g)(\mu_{en}/\rho)_a}, \qquad (3)$$

where, $(\mu_{en}/\rho)_g$ and $(\mu_{en}/\rho)_a$ are the mass energy absorption coefficients for glandular and adipose tissue, respectively, for the given energy. The unit of the constant 1.8352×10^{-17} is (mGy g)/keV.

Using the recent mass energy attenuation coefficients of photons through air, provided by NIST laboratory [14], a Monte Carlo-based simulation program was tailored for calculating absorbed energy in the breast model for a given configuration of breast tissue composition, thickness and for monoenergetic photon beam. Then, an additional procedure was added to that program, in order to compute the $G(E)$ factor during the simulation run-time, which in turn outputs the $DgN(E)$ coefficients for each studied case.

The Geant4-based simulation program was tailored to model monochromatic X-ray emission from a "point-like" source and to follow particle transportation through the breast. The physical processes used were the photoelectric effect, the Compton and the Rayleigh scattering for photons and the bremsstrahlung, the ionization and the "multiple scattering" for electrons. The production thresholds were set to 1 keV for photons and 10 keV for electrons. From the existing suite of physical packages, ready to use within the simulation program, the "PhysListEmStandard" was selected. Elemental compositions of adipose, glandular and skin tissue were based on the work of Ref. [27].

For each set of (monoenergetic) X-ray energy, breast size and breast composition, a simulation run was executed using 10^6 entrant photons providing sufficient statistical precision. In order to simplify analytical form of the fitting functions to be used and due to the small contribution to *MGD* parameters, we omitted the interval of energy of 1–11 keV during the fitting stage of the database. Notice that such contribution does not exceed 1% of the *MGD* for the studied X-ray spectra. $DgN(E)$ coefficients for 11–120 keV X-rays were computed. At least a total number of 1582 (113×7×2) runs were carried out for the data-base generation purpose covering 113 energy values (11–120 keV), and seven thicknesses (2–8 cm) for glandularities of 100% and 50%. The absorbed dose by the breast tissue was recorded for direct derivation of the $DgN(E)$ coefficients (in the SI units of mGy/mGy).

As we followed the same simulation setup used by Boone *et al.* [11], the same source-to-detector distance of 60 cm was used. Changing the distance to 80 cm or 40 cm can deviate the beam energy at the vicinity of the breast by less than 1%, which is logical due to the fact that the addition or subtraction of a 20 cm layer of air medium can affect the primary beam trajectory by 0.4% and 0.06% for 30 keV and 100 keV photon energy, respectively. Moreover, the assumption of modeling the geometry of the X-ray tubes focal spot as a point-like rather than a disc is valid to about 1%. The replacement of a point-like source with a disc of Φ40 μm or Φ300 μm (as found in clinical realistic tests), deviate the $DgN(E)$ with 0.213% or 0.444% for a given couple of photon energy, glandularity and thickness of (50 keV, 50%, 2 cm) or (10 keV, 100%, 8 cm), respectively. Whereas the focal spot size affects contrast of the images [28].

We can consider the homogeneous distribution of the glandular tissues within the breast as a limitation of the current model, as mentioned by Dance *et al.* [29] that the absorbed energy by the glandular tissue depends on the glandular tissue position in the breast.

The simulation was carried out using Geant4 (V9.4.p01) under a Red Hat Enterprise Linux 5 workstation on an Intel Core i7 (CPU) running with a 4 GB RAM at 3.40 GHz. The statistical uncertainty (2σ) associated with all the Monte Carlo calculations presented in this work is less than 1%.

B.   Parameterization procedure

The following parameterization procedure was followed to reduce the large amount of $DgN(E)$ values while retaining the prediction precision to an acceptable level of accuracy and us-ing simple analytical form of the fitting equation. For accuracy of the proposed method, the r^2 statistical coefficient value was calculated. We fitted the overall data set of $DgN(T,E)$ using Eq. (4) for the energy interval of 11–120 keV, for glandularities of 100% and 50% separately

$$DgN(E) = \frac{a + c\ln(T) + e\ln(E) + g\ln^2(T) + i\ln^2(E) + k\ln(T)\ln(E)}{1 + b\ln(T) + d\ln(E) + f\ln^2(T) + h\ln^2(E) + j\ln(T)\ln(E)}. \qquad (4)$$

And the *MGD* was calculated using Eq. (5):

$$MGD = \frac{\sum_{E_{\min}}^{E_{\max}} K(E) \times DgN(E) \times (E) \times \phi(E)}{\sum_{E_{\min}}^{E_{\max}} K(E) \times \phi(E)}, \qquad (5)$$

where, $\phi(E)$ is the photon fluence per exposure in units of mR per photons per mm^2 and $E_{\min}$ and $E_{\max}$ are the minimum and the maximum energy spectrum limits.

Physically spoken, it is clear from Eq. (4) that any DgN coefficient explicitly depends on the coming photon energy and the breast phantom thickness [30]. Thus, we prefer to fit those values with a bi-variant polynomial depending on E and T [13]. The quotient form can be explained by the fact that the DgN coefficient is a fraction of the absorbed dose by the breast model to the air medium, and each of them can be a polynomial energy dependent function. For a relative difference between computed and fitted values that does not exceed 3% on the *MGD* calculation for the majority of X-ray beam spectra. We were limited to adopt the second order polynomial fitting Eq. (4). More precision needs extension to higher order, with the penalty of complicating the fitting expression form.

To our knowledge, fitting methods using the parameter E was treated similarly by many authors [7, 26, 30], whereas the introduction of the parameter T as a second variable within its actual form is proposed for the first time herein.

III.   RESULTS AND DISCUSSION

We started with studying effects of photon fluence per exposure coefficient which, in turn, caused the modification in DgN value between those of Boone *et al.* [11] and those presented during this work. Moreover, the fitting parameters were tabulated for any easy handling of the computational model.

Based on the parameterization procedure, we studied the efficiency to reproduce directly simulated *MGD* for some specific cases. We terminated this work with analyzing the interpolation and the extrapolation capabilities of such procedure. Further work can be conducted towards the use of heterogeneous breast tissue composition and within a prone breast situation.

A.   X-ray Quanta per mm^2 per mR computation

We calculated the photon fluence per exposure conversion coefficient, using Eq. (1), for photon energy of 1–120 keV. Figure 1 shows the relative difference between $K(E)$ calculated based on the most recent data of mass energy absorption coefficient of air, provided by NIST [14], and those tabulated by Boone *et al.* [26]. The major difference seen concerns photons with energy lower than 75 keV and can reach 12% for 27 keV, as seen in the inset. For photon energies over 75 keV, such difference does not exceed 1%.
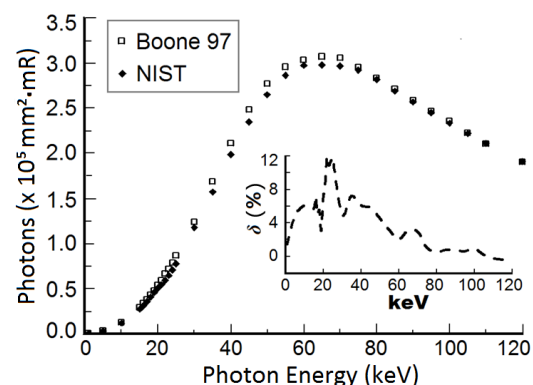

Fig. 1. Comparison of the photon quanta per mm^2 per mR parameter calculated in this work (denoted by NIST) against Boone *et al.* [26] data (denoted by Boone 97). The inset refers to their relative deviation as function of the energy.

B. $K(E)$ variation effect on Boone's look-up table

Table 1 illustrates a comparison of *MGD* calculations between literature (Boone *et al.* [5]) and present study using the updated $K(E)$ values. The comparison concerns three different anode/filter combinations of Mo/Mo (30 μm), W/Rh (50 μm) and W/Pd (50 μm) for 23–35 kVp and HVL of 0.269–0.597 mm of Al. The breast thickness was 4 cm and the glandularity was 50%. We observed a maximum relative difference between literature and Geant4 data of about 1.9, 5.0 and 4.2%, and between calculated (parameterized) and Geant4 data of about 2.6, 3.8 and 4.1%, respectively, for the above anode/filter combinations.

TABLE 1. *MGD* (mGy/mGy) calculated for different combinations of anode/filter, kVp and *HVL*: using Boone's method (denoted by Boone *et al.* [5]), directly simulated using Geant4 (denoted by G4) and using the parameterization method (denoted by Calc.). Deviation between Boone *et al./Calc.* and G4 data were tabulated in %

| Anode/filter	E	HVL	MGD			Deviation (%)	
	(kVp)	(mm Al)	Boone *et al.* [5]	G4	Calc.	Boone *et al.* [5]	Calc.
Mo/Mo30	23	0.269	0.158	0.155	0.151	1.935	2.581
	25	0.295	0.179	0.178	0.175	0.562	1.685
	27	0.318	0.195	0.197	0.195	1.015	1.015
	29	0.338	0.210	0.212	0.212	0.943	0.000
	31	0.356	0.222	0.225	0.225	1.333	0.000
	33	0.372	0.233	0.236	0.237	1.271	0.424
	35	0.386	0.243	0.244	0.246	0.410	0.820
W/Rh50	23	0.420	0.258	0.265	0.266	2.642	0.377
	25	0.462	0.289	0.299	0.302	3.344	1.003
	27	0.489	0.307	0.321	0.326	4.361	1.558
	29	0.509	0.321	0.338	0.349	5.030	3.254
	31	0.527	0.332	0.349	0.358	4.871	2.579
	33	0.544	0.344	0.358	0.371	3.911	3.631
	35	0.560	0.355	0.370	0.384	4.054	3.784
W/Pd50	23	0.424	0.260	0.267	0.269	2.622	0.749
	25	0.478	0.300	0.309	0.312	2.913	0.971
	27	0.514	0.324	0.337	0.341	3.858	1.187
	29	0.539	0.340	0.355	0.367	4.225	3.380
	31	0.560	0.353	0.366	0.377	3.552	3.005
	33	0.579	0.365	0.377	0.392	3.183	3.979
	35	0.597	0.377	0.389	0.405	3.085	4.113
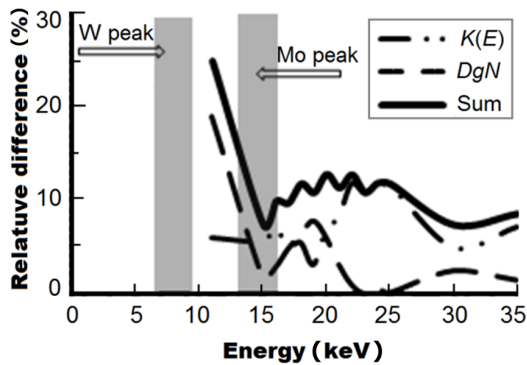
Fig. 2. Relative difference curves of $DgN(E)$, $K(E)$ and their sum vs. E, between those computed in this work to those derived using old cross section data-base and Monte Carlo simulation code found by Boone *et al.* [5, 22]. The two energy intervals (grey bands) indicate the localization of the main peak of the tungsten (W) and the molybdenum (Mo) experimental spectra.

TABLE 2. Computer-fit parameters used to derive $DgN(E,T)$, in mGy/mGy, for $E = 11$–120 keV and $T = 2$–8 cm. f_g: glandularity, p: (a, .., k). The statistical p-value (r^2) was given

p	$f_g = 100\%$	$f_g = 50\%$
a	−0.1463	−0.1811
b	0.01196	0.006104
c	0.1547	0.1986
d	−0.5080	−0.5147
e	−0.03587	−0.04615
f	0.03782	0.04211
g	0.03284	0.0359
h	0.09141	0.09939
i	0.05131	0.06342
j	−0.05943	−0.06876
k	−0.1040	−0.1269
r^2	0.9999	0.9999

will be lower than those for the molybdenum, for the studied kVp interval.

Referring to the Mo and W experimental spectra in [31], we observed that the two characteristic peaks were located around 17 keV and 11 keV, respectively, as shown in Fig. 2. The spectra covered 23–35 kVp. Also, Fig. 2 illustrates the curves of the relative error (%) of $K(E)$, $DgN(E)$ and their sum. According to Eq. (5) and Fig. 2, we are intended to find the *MGD* relative difference corresponding to the tungsten anode twice or higher than those for molybdenum. This can be explained by coincidence of the tungsten peak and the maximum relative deviation. Furthermore, we can guess that the relative deviation corresponding to the rhodium anode spectra

C. Data set generation and parameterization

The overall normalized glandular dose data were generated using Eqs. (2) and (3) and the developed simulation code, for breast glandularities of 100% and 50%. The data set corresponding to $f_g = 50\%$ is shown in Fig. 3. Plots corresponding to $f_g = 100\%$ are similar to Fig. 3. Table 2 illustrates the parameters resulting from fitting the overall DgN values and using Eq. (4) for energy interval of 11–120 keV. There is no

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TABLE 3. $DgN(E)$ coefficients, in mGy/mGy, directly simulated (denoted by G4) and parameterized (denoted by Calc) for different glandularity values of 20%, 40%, 60%, 80% and 90 %. E: energy in keV, T: thickness in cm

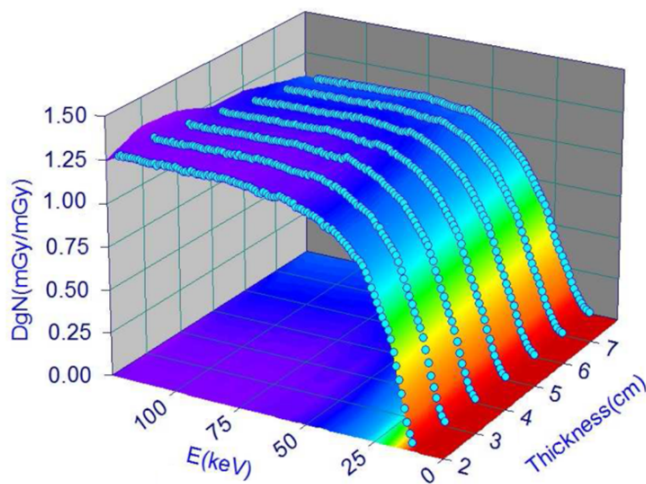| E(keV)	T(cm)	$f_g = 20\%$		$f_g = 40\%$		$f_g = 60\%$		$f_g = 80\%$		$f_g = 90\%$	
		G4	Calc.	G4	Calc.	G4	Calc.	G4	Calc.	G4	Calc.
15	2	0.34	0.34	0.32	0.32	0.30	0.30	0.28	0.29	0.28	0.28
50	2	1.20	1.19	1.21	1.20	1.21	1.20	1.22	1.21	1.23	1.21
15	4	0.18	0.18	0.17	0.17	0.15	0.15	0.14	0.14	0.13	0.13
50	4	1.18	1.19	1.19	1.19	1.18	1.19	1.19	1.19	1.20	1.19
15	8	0.09	0.09	0.08	0.08	0.07	0.07	0.07	0.07	0.06	0.06
50	8	1.03	1.03	1.03	1.02	1.02	1.02	1.02	1.01	1.02	1.01

Fig. 3. (Color online) Simulated DgN (mGy/mGy) versus energy (keV) and thickness (cm) for 50% glandularity, generated using the Geant4-based simulation program.

need to subdivide the energy and thickness intervals, for parameterization purposes. A statistical test p-value of 0.9999 was seen for both cases.

D.   *MGD* prediction ability

In order to investigate the possibility of *MGD* prediction using the current data set of DgN following the fitting method, we used Eq. (5) and the photon fluence per exposure spectrum corresponding to the anode/filter combinations of: Mo/Mo (30 µm), W/Rh (50 µm) and W/Pd (50 µm) generated according to the MASMIP and the TASMIP Boone's codes [26] for different kVp and HVL X-ray tube parameters. The heel effect associated to the spectra was not taken into account for this study, similar to [16]. Thus the beam is assumed to have a uniform intensity and uniform spectral quality within the field covering the entire breast. If we took it into account, the *MGD* would vary as it is proportional to the fluence spectra.

From the data at 35 kVp in Table 1, we can see that *MGD* values become close to each other. This is due to the small contribution of DgN for low photon energy and high kVp. The results are in acceptable agreement with those directly simulated.

E.   Interpolation and extrapolation capability

The DgN data values in Table 3 demonstrate effectiveness of the interpolation and extrapolation procedures, in terms of glandularity. The direct calculation using the linear interpolation and extrapolation technique and the Monte Carlo simulation were conducted for different cases of glandularity and the data are tabulated. We find an acceptable agreement between the two sets of data allowing the straightforward interpolation and extrapolation of the *MGD* for any given glandularity from about 0% to 100%.

IV.   CONCLUSION

We calculated the photon fluence per exposure conversion coefficient, using Eq. (1), for the interval of photon energy ranging from 1 keV to 120 keV. A computer simulation program was developed to estimate the radiation dose to the breast phantom during quality control and quality assurance Mammography tests. Monoenergetic DgN coefficients were computed for various energies and thicknesses and the data have been parameterized and presented in the form of a general equation and parameters depending on the two variables of E and T. The Geant4-based computed DgN coefficients presented in this work provide an update version of those maintained during mammographic dosimetry quality control tests, nowadays. The ultimate need to recompute such coefficients is related to any update occurring to the mass-energy absorption data-base of materials, which in turn influences any Monte Carlo simulation outputs. Even though that the relative difference found during the calculation of the $K(E)$ parameter reached 12% for 27 keV, the relative difference occurring to the *MGD* values attained the 5% for the studied cases of Molybdenum and Tungsten anode spectra. The parameterization procedure allowed us to correctly compute the *MGD* values for any X-ray spectra. Using the linear interpolation and extrapolation techniques, we are able to vary the kVp up to 120 keV, the breast phantom thickness from 2 cm to 8 cm and the glandularity proportion from about 0% to 100% and correctly reproduce *MGD* values derived from direct simulation. Such parameterization procedure can be straightforwardly applied to modern techniques such as breast CT and digital breast tomosynthesis, despite compressed breast CT in concern.

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